

Poisson integrators

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Abstract

An overview of Hamiltonian systems with noncanonical Poisson structures is given. Examples of bi-Hamiltonian ode's, pde's and lattice equations are presented. Numerical integrators using generating functions, Hamiltonian splitting, symplectic Runge-Kutta methods are discussed for Lie-Poisson systems and Hamiltonian systems with a general Poisson structure. Nambu-Poisson systems and the discrete gradient methods are also presented.

Keywords: Hamiltonian ode's and pde's, symplectic integrators, Lie-Poisson systems, bi-Hamiltonian systems, integrable discretizations, Nambu-Hamiltonian systems.

1 Introduction

In this review article we present Hamiltonian systems with a non-canonical Poisson structure and give an overview of Poisson structure preserving numerical integrators. In the last decade, efficient and reliable numerical integrators were constructed for canonical Hamiltonian systems with symplectic structure (see [26, 51]). The theoretical foundation of stability and convergence of symplectic integrators was provided by the backward error analysis [26]. Methods based on the preservation of the geometric features of the continuous system by discretization are called "geometric integrators", which include also the symplectic methods (see for a state of art review of these methods and their applications [10]). They have better stability properties, smaller local and global errors than the standard integrators based on the

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local error control. The quadratic invariants of the underlying continuous system are exactly preserved by symplectic integrators. Complicated invariants, among them the polynomial invariants of order three and greater are in general not preserved ([10], [26]). The phase space structure of low dimensional Hamiltonian systems are very accurately preserved by symplectic methods. But the applicability of symplectic integrators for higher dimensional systems arising from semidiscretization of Hamiltonian pde's is not well established [1].

The noncanonical Hamiltonian systems on Poisson manifolds arise in many applications. The best known example is the Euler top equation, a three dimensional Hamiltonian system. The Poisson structure is more general than the symplectic structure, the dimension of a Poisson manifold doesn't need to be even as in the case of the Euler top equation compared to symplectic manifolds which appear only in even dimensions. The Poisson systems occur as finite dimensional systems in the form of ode's and nonlinear lattice equations or as infinite dimensional systems in the form of pde's. Hamiltonian pde's like the Korteweg deVries (KdV) equation, the nonlinear Schrödinger equation (NLS) and Euler equations of an incompressible fluid have many applications in hydrodynamics, optics and meteorology. The algebraic and geometric properties of the Poisson manifolds, like the Poisson bracket, Darboux transformations, Casimirs, symplectic foliation and integrability, are given in Section 2. Many Hamiltonian systems can be written with respect to the same coordinate system in more than one Hamiltonian formulation. The so called bi-Hamiltonian systems occur as ode's, pde's and in nonlinear lattices. The properties of bi-Hamiltonian systems, and finite dimensional examples are given in Section 3. The real application of the bi-Hamiltonian formulation is the field of Hamiltonian pde's and nonlinear lattice equations, which are presented in Section 4.

Geometric integrators for noncanonical Hamiltonian systems or Poisson systems are largely unexamined. There exist a variety of methods for the Lie-Poisson systems, Hamiltonian systems with a linear Poisson structure. The generating function approach [13] and splitting methods based on the separability of Hamiltonian for canonical Hamiltonian systems were extended to the Lie-Poisson systems [34]. Unfortunately there exists no general method for Hamiltonian systems with a general Poisson structure beyond the Lie-Poisson integrators. One can show that some of the symplectic methods for canonical Hamiltonian systems may preserve the Poisson structure of some Hamiltonian systems. This means that whether an integrator is Poisson or not, depends on the specific problem. For some nonlinear lattice equations, it is possible by using the Darboux coordinates to transform the Hamiltonian system with the Poisson structure to a canonical one and then integrate this system by the symplectic methods. But there exists no

general algorithm for such a transformation. These aspects of Poisson integrators are discussed in Section 5.

In Section 6 the so called Nambu-Hamilton systems which can be considered as an extension of the Poisson structure are presented. The structure of these systems is discussed and the discrete gradient methods which applicable for them, are described.

2 Poisson structures and Hamiltonian systems

In order to present the finite dimensional and infinite dimensional Hamiltonian systems, we have to look at the properties of the Poisson manifolds and functions defined on these manifolds. In our presentation we follow mainly [41], Chapters 6 & 7. The key property here is the so called Poisson bracket, which assigns to each pair of functions F and G in the space of smooth functions $\mathcal{F}(\mathcal{M})$ on a smooth manifold \mathcal{M} a third function, denoted by $\{F, G\}$.

Definition 1 *The Poisson bracket is a bilinear operation satisfying the following conditions:*

(i) *skew-symmetry*

$$\{F, G\} = -\{G, F\},$$

(ii) *the Leibniz rule*

$$\{F, G \cdot P\} = \{F, G\} \cdot P + G \cdot \{F, P\},$$

(iii) *the Jacobi identity*

$$\{\{F, G\}, P\} + \{\{P, F\}, G\} + \{\{G, P\}, F\} = 0,$$

where \cdot denotes the ordinary multiplication of functions.

A manifold \mathcal{M} with a Poisson bracket is called a Poisson manifold and the bracket defines a Poisson structure on \mathcal{M} . The Poisson manifold is more general than a symplectic manifold; it doesn't need to be even dimensional. The canonical Poisson bracket on a even dimensional Euclidean space $\mathcal{M} = \mathbb{R}^m$, $m = 2n$ with the canonical coordinates $(p, q) = (p_1, \dots, p_n, q_1, \dots, q_n)$ is given for two smooth functions $F(p, q)$ and $G(p, q)$ by

$$\{F, G\} = \sum_{i=1}^n \left(\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \right). \quad (1)$$

with the bracket identities

$$\{p_i, p_j\} = 0, \quad \{q_i, q_j\} = 0, \quad \{q_i, p_j\} = \delta_j^i, \quad i, j = 1, \dots, n$$

where δ_j^i denotes the Kronecker symbol.

The general local coordinate picture of a m dimensional Poisson manifold \mathcal{M} is given by the Poisson bracket on local coordinates $x = (x_1, \dots, x_m)$. The Poisson bracket for two smooth functions $F(x)$ and $G(x)$ takes the form

$$\{F, G\} = \sum_{i=1}^m \sum_{j=1}^m \{x_i, x_j\} \frac{\partial F}{\partial x_i} \frac{\partial G}{\partial x_j} \quad (2)$$

A Hamiltonian vector field X_H on \mathcal{M} with the coefficients functions $\xi_i(x)$ depending on H is given by

$$X_H = \sum_{i=1}^m \xi_i(x) \frac{\partial}{\partial x_i}$$

and satisfies

$$X_H(F) = \{F, H\} = -\{H, F\}.$$

The governing equations of the flow associated with the vector field are called Hamiltonian equations

$$\dot{x} = \{x, H\}. \quad (3)$$

Definition 2 *A general Hamiltonian system is given then by the triple \mathcal{M} , the manifold, $\{\cdot, \cdot\}$, the Poisson structure and $H(x)$ a real function on \mathcal{M} . The Poisson structure gives the coordinate functions $J_{ij} = \{x_i, x_j\}$ which are called structure functions. They satisfy the Leibniz rule and have the following properties*

i) *skew-symmetry:*

$$J_{ij}(x) = -J_{ji}(x), \quad i, j = 1, \dots, m$$

ii) *Jacobi identity:*

$$\sum_{i=1}^m \{J_{il} \partial_l J_{jk} + J_{kl} \partial_l J_{ij} + J_{jl} \partial_l J_{ki}\} = 0, \quad i, j = 1, \dots, m \quad (4)$$

for all $x \in \mathcal{M}$ with $\partial_l = \partial/\partial x_l$.

The conditions for the Jacobi identity (4) form a system of nonlinear partial differential equations for the structure functions $J_{ij}(x)$. The structure functions can be assembled into a skew-symmetric structure matrix $J(x) \in \mathbb{R}^{m \times m}$. In this case the Poisson bracket (2) for the functions F and G takes the form

$$\{F, G\} = \nabla F(x)^T J(x) \nabla G(x)$$

and the Hamiltonian equation (3) can be rewritten as

$$\dot{x} = J(x)\nabla H(x).$$

The most important examples of Poisson structures are associated with m -dimensional Lie algebras. The associated Lie-Poisson bracket between two functions F, G with the structure constants c_{ij}^k , $i, j, k = 1, \dots, m$ of the Lie algebra, is given by

$$\{F, G\} = \sum_{j,k=1}^m c_{ij}^k x_k \frac{\partial F}{\partial x_i} \frac{\partial G}{\partial x_j}.$$

with the linear structure functions $J_{ij}(x) = \sum_{k=1}^m c_{ij}^k x_k$.

Example 1: Euler top equation

The most important example of a Lie-Poisson system

$$\frac{dx_i}{dt} = \sum_{j,k=1}^m c_{ij}^k x_k \frac{\partial H}{\partial x_j}, \quad i = 1, \dots, m$$

is the Euler top equation describing the motion of a rigid body around a fixed point:

$$\dot{x}_1 = \frac{I_2 - I_3}{I_2 I_3} x_2 x_3, \quad \dot{x}_2 = \frac{I_3 - I_1}{I_3 I_1} x_3 x_1, \quad \dot{x}_3 = \frac{I_1 - I_2}{I_1 I_2} x_1 x_2 \quad (5)$$

where I_1, I_2, I_3 denote the moments of inertia. The Poisson structure is given by

$$\{x_1, x_2\} = -x_3, \quad \{x_2, x_3\} = -x_1, \quad \{x_3, x_1\} = -x_2 \quad (6)$$

It can be written in the Hamiltonian form (3) with the energy integral H as the Hamiltonian

$$H = \frac{1}{2} \left(\frac{x_1^2}{I_1} + \frac{x_2^2}{I_2} + \frac{x_3^2}{I_3} \right) \quad (7)$$

and with the linear structure matrix

$$J(x) = \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix},$$

$$\frac{dx}{dt} = J(x)\nabla H(x) = x \times \nabla H(x)$$

here \times denotes the cross product.

Theorem 1 *A Poisson manifold of dimension m is symplectic if the rank of the Poisson structure is maximal everywhere. Because the rank of a Poisson manifold at any point is always an even integer, a symplectic manifold is necessarily even dimensional. In other words if the structure matrix $J(x)$ is invertible, then according to Darboux's theorem the Poisson structure is isomorphic to the standard symplectic structure in \mathbb{R}^{2n} . In this case the structure matrix $J(x)$ determines a symplectic structure on $\mathcal{M} \subset \mathbb{R}^m$, $m = 2n$ if and only if its inverse $K(x) = J(x)^{-1}$ satisfies the following conditions ([41], Proposition 6.15)*

i) *skew-symmetry:*

$$K_{ij}(x) = -K_{ji}(x), \quad i, j = 1, \dots, m$$

ii) *Jacobi identity:*

$$\partial_k K_{ij}(x) + \partial_j K_{ki}(x) + \partial_i K_{jk}(x) = 0, \quad i, j, k = 1, \dots, m$$

The nonlinear partial differential equations for the structure functions in the Jacobi identity (4) simplify to linear partial differential equations involving $K_{ij}(x)$.

Definition 3 [41] *A Poisson structure is called degenerate, if the structure matrix $J(x)$ is non-invertible. It follows from the skew-symmetry that the rank of the Poisson matrix at any point is always an even integer, which implies that odd dimensional systems have a degenerate Poisson structure. If the manifold is of dimension $m = 2n + l$ and the rank of $J(x)$ is $2n$ everywhere, then there exist distinguished functions $F_i(x) = c_i, i = 1, \dots, l$, called Casimirs, whose Poisson bracket vanish with any function or variable x_i , i.e. $\{F_i(x), x_i\} = 0, i = 1, \dots, l$.*

If the Poisson structure is of constant rank, the symplectic foliation simplifies. One can introduce local coordinates, which bring the foliation to the canonical form, which results from the Darboux theorem ([41], Theorem 6.22). At each point $x \in \mathcal{M}$ of an m -dimensional manifold of constant rank $2n \leq m$ everywhere, the Darboux theorem says then, there exist local coordinates $(q_1, \dots, q_n, p_1, \dots, p_n, z_1, \dots, z_l)$ in terms of which the Poisson bracket takes the canonical form (1), where p_i, q_i denote the canonical variables. There exist locally l independent Casimirs $F_i(x), \dots, F_l(x)$; their common level surfaces $F_1(x) = c_1, \dots, F_l(x) = c_l$ are called symplectic leaves of the Poisson bracket. Using the Darboux transformation, the Poisson structure can be transformed on the symplectic leaves to the canonical one.

If the structure matrix $J(x)$ is constant and nonsingular in some coordinate systems, then a linear change of coordinates reduces the

Poisson structure to the canonical one [17]. The reduction of the Poisson structure using Casimirs on symplectic leaves produce usually more complicated systems. For example for the Euler top equations, the total angular momentum

$$I = \frac{1}{2}(x_1^2 + x_2^2 + x_3^2), \quad (8)$$

is a Casimir (commutes with $x_i, i = 1, \dots, 3$) and the symplectic leaves are the spheres described by (8). Using the transformations

$$q = \arccos\left(\frac{x_1}{(x_1^2 + x_2^2)^{1/2}}\right), \quad p = x_3$$

the Euler top equation can be reduced to a canonical Hamiltonian system ([9], pp. 7)

$$H(q, p, c) = (I - p^2) \left(\frac{1}{I_1} \cos^2 q + \frac{1}{I_2} \sin^2 q \right) + \frac{p^2}{I_3}.$$

The geometric characterization of the local and global structure of Poisson manifolds is given by the splitting theorem of Weinstein [52]:

Theorem 2 *On a Poisson manifold \mathcal{M} , any point $x \in \mathcal{M}$ has a coordinate neighborhood with coordinates $q_1, \dots, q_k, p_1, \dots, p_k, y_1, \dots, y_l$ centered at x , such that*

$$\Pi = \sum_i \frac{\partial}{\partial q_i} \wedge \frac{\partial}{\partial p_i} + \sum_{i,j} \varphi_{ij}(y) \frac{\partial}{\partial y_i} \wedge \frac{\partial}{\partial y_j}, \quad \varphi_{ij}(0) = 0. \quad (9)$$

This theorem gives a decomposition of the neighborhood of x as the product of two Poisson manifolds: one with rank $2k$ and the other with rank 0 at x . The local structure of a Poisson manifold is described by the symplectic leaves and their transverse Poisson structures (the second part in 9). Globally, a Poisson manifold is obtained by gluing together the symplectic manifolds. There are three special cases of the splitting theorem [52]:

- *If the rank is locally constant, then $\varphi_{ij} = 0$. The splitting theorem reduces to the Lie's theorem, i.e. each point of \mathcal{M} is contained in a local coordinate system with respect to which the structure functions J_{ij} are constant*
- *At the origin of \mathcal{M} one has only y_i 's, the first term in (9) does not appear.*
- *A symplectic manifold is a Poisson manifold where rank $\Pi = \dim \mathcal{M}$ everywhere. The splitting theorem gives canonical coordinates $q_1, \dots, q_k, p_1, \dots, p_k$.*

There exists a close relation between the symmetries and conservation laws of Hamiltonian systems. Noether's theorem provides a connection between the symmetries and conservation laws or first integrals and can be applied to Hamiltonian systems. The first integrals are characterized by the vanishing of the Poisson bracket: a function \mathcal{I} is a first integral of the autonomous Hamiltonian system (3), if $\{\mathcal{I}, H\} = 0$ for all $x \in \mathcal{M}$. A Hamiltonian system with a time-independent Hamiltonian has $H(x)$ as the first integral. The Casimirs $F_i(x)$ determined by the Poisson structure $J(x)$ are first integrals too, but they arise from the degeneracies of the Poisson bracket and are not generated by the symmetry properties of the Hamiltonian system. If the Poisson manifold is symplectic, only constant functions are Casimirs.

Hamiltonian systems are usually non-integrable, there are in general no additional integrals of motion. But there is a class of Hamiltonians which are called completely integrable.

Definition 4 [48] *A Hamiltonian system is called completely integrable if it has n integrals of motion $I_k(q, p), k = 1, \dots, n$*

- *which do not depend explicitly on time,*
- *are functionally independent, i.e.*

$$\text{rank} \left(\frac{\partial I_k}{\partial q_j}, \frac{\partial I_k}{\partial p_j} \right)_{k,j=1,\dots,n} = n,$$

- *are in involution*

$$\{I_j, I_k\} = 0 \quad \text{for each pair } (j, k), \quad j, k = 1, \dots, n.$$

The Liouville theorem then says that any integrable system can be integrated by quadratures. The geometric content of complete integrability is described by the Liouville-Arnold theorem:

Theorem 3 [17, 44, 48] *If the surface of the constant value of the Hamiltonian $H(q, p) = E$ is compact connected manifold, then*

- *the manifold*

$$\mathcal{M} = \{(q, p) : I_k(q, p) = c_k = \text{const}, \quad k = 1, \dots, n\}$$

diffeomorphic to the torus T^n ,

- *in the canonically conjugate action and angle coordinates (I_k, φ_k) , Hamilton equations have a simple form:*

$$\dot{\varphi}_i = \omega_k(I), \quad \dot{I}_k = 0, \quad k = 1, \dots, n,$$

- the action-angle variables have a simple dependence on time

$$I_k(t) = \text{const}, \quad \varphi_k(t) = \varphi_k^{(0)} + \omega_k t,$$

the variable φ_k determines the position of a point on the torus and vary linearly with time; the motion is quasiperiodic on the torus T^n ,

- the Hamilton equations can be solved by quadratures.

The Euler top equation is completely integrable. Other examples of completely integrable rigid body equations are the Lagrange top, and the Kowalevskaya top equations [4].

If a Hamiltonian system has $2n - 1$ independent integrals at most, it is called completely degenerate. Such systems occur in very rare cases for Hamiltonian with a potential function $V(q) = \alpha/q$ for the Kepler problem, $V(q) = \frac{1}{2}q^2$ for the harmonic oscillator and for the Calogero-Moser system [48].

3 Bi-Hamiltonian systems

Definition 5 A system of differential equations is called bi-Hamiltonian if it can be written in the Hamiltonian form in two distinct ways [42] :

$$\frac{dx}{dt} = J_0(x)\nabla H_1 = J_1(x)\nabla H_0 \quad (10)$$

with the structure matrices $J_0(x)$ and $J_1(x)$ determining the Poisson bracket $\{F, G\}_k = \nabla F^T J_k(x) \nabla G$, $k = 0, 1$. The structure defined by $J_0(x)$ and $J_1(x)$ is called a Hamiltonian pair.

A Hamiltonian pair is compatible, if the linear combination of $J_1(x) - \lambda J_0(x)$ determines also a Poisson bracket for any real λ . The compatibility condition is not trivial, because the differential equations must be satisfied for the Jacobi identity (4). In the symplectic case (non-degenerate $J_k(x)$, $k = 1, 2$ and n is even), the Jacobi conditions can be replaced by the symplectic two-forms

$$\Omega_k = \frac{1}{2} dx \wedge K_k(x) dx, \quad K_k(x) = J_k^{-1}(x), \quad k = 0, 1$$

which are closed, i.e. $d\Omega_k = 0$. For a given pair, the corresponding Hamiltonian system can be found by solving the linear system of partial differential equations $\nabla H_1 = J_1^{-1}(x) J_0(x) \nabla H_0$ [40]. A Hamiltonian pair is called non-degenerate at the point x if the skew-symmetric matrix pencil $J_\lambda(x) = J_1(x) - \lambda J_0(x)$ is nonsingular for at least one finite λ . According to Magri [32] bi-Hamiltonian systems with a compatible Hamiltonian pair are completely integrable.

Theorem 4 *For any bi-Hamiltonian system with a non-degenerate, compatible bi-Hamiltonian structure, there exists a hierarchy of Hamiltonian functions H_0, H_1, H_2, \dots , all in involution w.r.t. both Poisson brackets $\{H_i, H_j\}_k = 0, k = 1, 2, i, j = 0, \dots$ and generating mutually commuting bi-Hamiltonian flows ([32, 42]), i.e. they are completely integrable. The sequence of first integrals can be constructed for bi-Hamiltonian systems by the Lenard recursion scheme ([4, 9, 17, 32]):*

$$\begin{aligned} \{\cdot, H_0\}_0 &= 0 & H_0 \text{ is a Casimir with respect to } \{\cdot, \cdot\}_0 \\ \{\cdot, H_1\}_0 &= \{\cdot, H_0\}_1, \\ \{\cdot, H_2\}_0 &= \{\cdot, H_1\}_1, \\ &\dots & \dots & \dots \\ \{\cdot, H_{k+1}\}_0 &= \{\cdot, H_k\}_1 \end{aligned}$$

which generate a sequence of bi-Hamiltonian vector fields

$$\begin{aligned} X_k &= \{x, H_k\}_0, \\ &= \{x, H_{k-1}\}_1, \quad k = 1, 2, \dots \end{aligned}$$

In case of infinite dimensional systems (pde's), one has an infinite number of first integrals. For finite dimensional systems, the Lenard recursion is either finite or infinite, in the second case only a finite number of integrals are linearly independent [9].

Example 2: Euler top equation as bi-Hamiltonian system

The Euler top equation (5) is also bi-Hamiltonian with respect to the second Poisson bracket

$$\{x_1, x_2\} = \frac{x_3}{I_3}, \quad \{x_2, x_3\} = \frac{x_1}{I_1}, \quad \{x_3, x_1\} = \frac{x_2}{I_2} \quad (11)$$

with the total angular momentum (8) as the second Hamiltonian. The corresponding structure matrix is given by

$$J_1(x) = \begin{pmatrix} 0 & \frac{x_3}{I_3} & -\frac{x_2}{I_2} \\ -\frac{x_3}{I_3} & 0 & \frac{x_1}{I_1} \\ \frac{x_2}{I_2} & -\frac{x_1}{I_1} & 0 \end{pmatrix}.$$

Examples of finite dimensional Hamiltonian systems with Poisson and bi-Hamiltonian structures are given in [25], [44].

Example 3: Lotka-Volterra equations

Three dimensional Lotka-Volterra system of competing species has a bi-Hamiltonian structure

$$\dot{x} = \begin{pmatrix} 0 & -x_1x_2 & x_1x_3 \\ x_1x_2 & 0 & -x_2x_3 \\ -x_1x_3 & x_2x_3 & 0 \end{pmatrix} \nabla H_1 = \begin{pmatrix} 0 & x_1x_2x_3 & -x_1x_2x_3 \\ -x_1x_2x_3 & 0 & x_1x_2x_3 \\ x_1x_2x_3 & -x_1x_2x_3 & 0 \end{pmatrix} \nabla H_2 \quad (12)$$

with the Hamiltonians

$$H_1 = x_1 + x_2 + x_3 \quad \text{and} \quad H_2 = \log(x_1) + \log(x_2) + \log(x_3). \quad (13)$$

Example 4: Lorenz system

$$\begin{aligned} \dot{x}_1 &= \sigma(x_2 - x_1) \\ \dot{x}_2 &= (\rho x_1 - x_1 x_3 - x_2) \\ \dot{x}_3 &= (-\beta x_3 + x_1 x_2) \end{aligned} \quad (14)$$

has a chaotic behavior for most values of the parameters. It is Hamiltonian with the following parameter values and the Hamiltonian

$$\rho = 0, \quad \sigma = \frac{1}{2}, \quad \beta = 1, \quad H = \frac{x_2^2 + x_3^2}{(x_1^2 - x_3)^2}.$$

with respect to the Poisson structure

$$\{x_1, x_2\} = x_1^2 x_3 + x_2^2, \quad \{x_2, x_3\} = -2(x_2^2 + x_3^2)x_1, \quad \{x_3, x_1\} = (x_1^2 - x_3)x_2.$$

The system has two time-dependent conserved quantities. Using a transformation of the dynamical variables and time, the equation (14) takes a bi-Hamiltonian form [25]

$$u'_1 = \frac{1}{2}u_2, \quad u'_2 = -u_1 u_3, \quad u'_3 = u_1 u_2.$$

with the Hamiltonians $H_1 = u_3 - u_1^2$, $H_2 = u_2^2 + u_3^2$ and with the corresponding Poisson brackets

$$\begin{aligned} \{u_1, u_2\}_0 &= \frac{1}{4}, \quad \{u_2, u_3\}_0 = -\frac{1}{2}u_1, \quad \{u_1, u_3\}_0 = 0, \\ \{u_1, u_2\}_1 &= \frac{1}{2}u_3, \quad \{u_2, u_3\}_1 = 0, \quad \{u_1, u_3\}_1 = \frac{1}{2}u_2 \end{aligned}$$

Other three dimensional systems admitting bi-Hamiltonian structure like the Halphen system, May Leonard equations, Maxwell-Bloch equations, and the Kermack-McKendrick model for epidemics are given in [25, 44].

There are few examples of bi-Hamiltonian systems in dimensions higher than three [9]. We give here as an example the Calogero-Moser system with two particles.

Example 5: Calogero-Moser system

The motion of repelling particles on a line is described by the Hamiltonian

$$H = \frac{1}{2} \sum_{j=1}^n p_j^2 + g^2 \sum_{j < k} \frac{1}{(q_j - q_k)^2}.$$

The four dimensional bi-Hamiltonian Calogero-Moser system for two particles is given in [32] with the Hamiltonians H_0 and H_1 .

$$H_1 = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{(q_1 - q_2)^2}, \quad H_0 = p_1 + p_2$$

$$\begin{aligned} \dot{x} &= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \nabla H_1 \\ &= \begin{pmatrix} 0 & \frac{2q_{12}}{4q_{12}^2 + p_{12}^2} & p_1 + \frac{2q_{12}^2 p_{12}}{4q_{12}^2 + p_{12}^2} & -\frac{2q_{12}^2}{4q_{12}^2 + p_{12}^2} \\ -\frac{2q_{12}}{4q_{12}^2 + p_{12}^2} & 0 & 0 & p_2 - \frac{2q_{12}^2 p_{12}}{4q_{12}^2 + p_{12}^2} \\ -p_1 - \frac{2q_{12}^2 p_{12}}{4q_{12}^2 + p_{12}^2} & 0 & 0 & 2q_{12}^3 \\ \frac{2q_{12}}{4p_{12}^2 + p_{12}^2} & -p_2 + \frac{2q_{12}^2 p_{12}}{4q_{12}^2 + p_{12}^2} & -2q_{12}^3 & 0 \end{pmatrix} \nabla H_0 \end{aligned}$$

where $q_{12} = \frac{1}{q_1 - q_2}$ and $p_{12} = p_1 - p_2$.

4 Bi-Hamiltonian pde's and lattice equations

Many nonlinear partial differential equations like the Korteweg de Vries (KdV) equation, the Euler equations of fluid dynamics and the nonlinear Schrödinger equation can be written in the Hamiltonian form. The Hamiltonian formulation for the ode's can be extended to pde's by replacing the Hamiltonian $H(x)$ by a Hamiltonian functional $\mathcal{H}[u]$, the gradient operation ∇H by the variational derivative $\delta \mathcal{H}$ and the skew-symmetric matrix $J(x)$ by a skew-adjoint differential operator $\Theta(\mathcal{D})$. The resulting Hamiltonian system has the form

$$\frac{\partial u}{\partial t} = \Theta(\mathcal{D}) \times \delta \mathcal{H}[u]$$

The right hand side of the Hamiltonian evolution equations

$$u_t = K[u] = K(x, u^{(n)})$$

contains the space variable vector x and $u^{(n)}$ represents all derivatives of the function $u(x, t)$ with respect to x of order at most n . The Poisson bracket between two functional \mathcal{F} and \mathcal{G} is defined by

$$\{\mathcal{F}, \mathcal{G}\} = \int \delta \mathcal{F} \cdot \Theta(\mathcal{D}) \mathcal{G} dx$$

which satisfies the skew-symmetry condition and the Jacobi identity. An interesting feature of the Hamiltonian pde's is that many of them

have a bi-Hamiltonian structure. As a result of this, there exists a hierarchy of mutually commuting Hamiltonian flows, and conserved quantities, generated by the recursion operator based on two compatible Poisson operators. In the last two decades the bi-Hamiltonian structures of many pde's were discovered, like the KdV equation, the nonlinear Schrödinger equations, the Euler equation, and the Boussinesq equation [41].

The Korteweg de Vries (KdV) equation has the bi-Hamiltonian form

$$\begin{aligned} u_t = u_{xxx} + uu_x &= D_x \delta \int \left(-\frac{1}{2}u_x^2 + \frac{1}{6}u^3 \right) dx = \Theta_0 \delta H_1(u) \\ &= \left(D_x^3 + \frac{2}{3}u D_x + \frac{1}{3}u_x \right) \delta \int \frac{1}{2}u^2 dx = \Theta_1 \delta H_0(u) \end{aligned}$$

The nonlinear Schrödinger (NLS) equation with the complex variable u

$$iu_t + u_{xx} + 2|u|^2 u = 0,$$

has the following bi-Hamiltonian structure [9]

$$\begin{aligned} \begin{pmatrix} u_t \\ u_t^* \end{pmatrix} &= \begin{pmatrix} iu_{xx} + 2iu|u|^2 \\ -iu_{xx}^* - 2iu^*|u|^2 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \delta \int_R (|u_x|^2 - |u|^4) dx \\ &= \begin{pmatrix} 2uD^{-1}u & -D - 2uD^{-1}u^* \\ -D - 2u^*D^{-1}u & 2u^*D^{-1}u^* \end{pmatrix} \delta \int_R \frac{1}{2}i(u_x^*u - u_xu^*) dx \end{aligned}$$

with u^* denoting the complex conjugate of u . Both systems, the KdV and NLS equations, possess due to their bi-Hamiltonian structure, infinitely many first integrals, i.e. they are completely integrable. The integrals can be generated using the Lenard scheme. If the differential operators Θ_0 and Θ_1 are compatible, the infinite hierarchy of bi-Hamiltonian systems is defined recursively by

$$u_t = \Theta_0 \delta H_{i+1} = \Theta_1 \delta H_i, \quad i = -1, \dots$$

with the integro-differential recursion operator $R = \Theta_1 \Theta_0^{-1}$ [3].

Nonlinear lattice equations or discrete nonlinear systems play an important role in modelling many physical phenomena. Examples of them are the Fermi-Pasta-Ulam lattice, the Toda and Volterra lattices, the Calogero-Moser system. They also arise by semi-discretization of some integrable nonlinear pde's like the Ablowitz-Ladik lattice which represents an integrable discretization of the nonlinear Schrödinger equation (4). Most of the nonlinear lattices are completely integrable.

The conserved quantities, the multi-Hamiltonian structure, the recursion operator, Lax form, and master symmetries of the lattice equations were investigated in recent years by many authors (see for example [15, 39]).

Example 6: Toda lattice

The motion of n interacting particles with an exponential interaction potential Hamiltonian

$$H = \sum_{i=1}^n \frac{1}{2} p_i^2 + e^{(q_i - q_{i+1})}$$

are described by the Toda lattice equations. Here the q_i 's denote the positions of the i -th particle and the p_i 's their momentum. Introducing the new variables $a_i = e^{(q_i - q_{i+1})}$, $b_i = p_i$ after Flaschka transformation, one obtains [45, 16]

$$\dot{a}_i = a_i(b_{i+1} - b_i), \quad \dot{b}_i = a_i - a_{i-1}, \quad 1 \leq i \leq n \quad (15)$$

with the open-end ($a_0 = a_n = 0$) or periodic ($a_0 = a_n$, $b_{n+1} = b_1$) boundary conditions. It has a tri-Hamiltonian structure with the following Poisson brackets and corresponding Hamiltonians [55]

- linear Poisson bracket (Lie-Poisson bracket):

$$\{b_i, a_i\}_1 = a_i, \quad \{a_i, b_{i+1}\}_1 = a_i$$

$$H_2 = \frac{1}{2} \sum_{i=1}^n b_i^2 + \sum_{i=1}^N a_i$$

- quadratic Poisson bracket:

$$\begin{aligned} \{b_i, a_i\}_2 &= a_i b_i, & \{a_i, b_{i+1}\}_2 &= a_i b_{i+1} \\ \{a_i, a_{i+1}\}_2 &= a_{i+1} a_i, & \{b_i, b_{i+1}\}_2 &= a_i \end{aligned}$$

$$H_1 = \sum_{i=1}^n b_i$$

- cubic Poisson bracket:

$$\begin{aligned} \{b_i, a_i\}_3 &= a_i(b_i^2 + a_i), & \{a_i, b_{i+1}\}_3 &= a_i(b_{i+1}^2 + a_i) \\ \{a_i, a_{i+1}\}_3 &= 2a_i a_{i+1} b_{i+1}, & \{b_i, b_{i+1}\}_3 &= a_i(b_i + b_{i+1}) \\ \{a_i, b_{i+1}\}_3 &= a_i a_{i+1}, & \{b_i, a_{i+1}\}_3 &= a_i a_{i+1} \end{aligned}$$

$$H_1 = \frac{1}{2} \sum_{i=1}^n \log(a_i)$$

With respect to the linear and quadratic Poisson brackets, the Toda lattice forms a bi-Hamiltonian system. Because both brackets are degenerate, it is not possible to find the recursion operator and apply the Lenard scheme to find the hierarchy of the integrals, which was done using master symmetries [16]. A different bi-Hamiltonian formulation of the Toda can be found in [16, 39]

Another interesting nonlinear lattice equation is the Volterra lattice [55] which is a model for vibrations of the particles on lattices (Liouville model on the lattice) and describes the population evolution in a hierarchical system of competing species. It can be also considered as an integrable discretization of Korteweg de Vries equations.

Example 7: Volterra lattice

$$\dot{y}_i = y_i(y_{i+1} - y_{i-1}), \quad i = 1, \dots, n \quad (16)$$

is bi-Hamiltonian

$$\dot{y} = J_0(y)\nabla H_1 = J_1(y)\nabla H_0$$

with respect to the quadratic and cubic Poisson brackets

$$\{y_i, y_{i+1}\}_0 = y_i y_{i+1}, \quad (17)$$

$$\{y_i, y_{i+1}\}_1 = y_i y_{i+1}(y_i + y_{i+1}), \quad \{y_i, y_{i+2}\}_1 = y_i y_{i+1} y_{i+2}. \quad (18)$$

and the corresponding Hamiltonians are

$$H_1 = \sum_{i=1}^n y_i, \quad H_0 = \frac{1}{2} \sum_{i=1}^n \log(y_i).$$

The Toda and Volterra lattices are closely related through the nonlinear transformation of variables [16]

$$a_i = y_{2i} y_{2i-1}, \quad b_i = y_{2i-1} - y_{2i-2}.$$

5 Lie-Poisson and Poisson integrators

It is natural to ask if the symplectic integrators applied to canonical Hamiltonian systems on symplectic spaces can be extended to produce integrators that preserve the linear Poisson structure (Lie-Poisson integrators) or the more general Poisson structures.

5.1 Integrators based on generating functions

The generating function approach in the framework of symplectic integrators was applied by several authors to Lie-Poisson systems. Ge and

Marsden constructed Lie-Poisson integrators in [24] by finding approximate solutions to the Hamilton-Jacobi Lie-Poisson equations using the generating functions developed in [13] for canonical Hamiltonian systems which is symplectic and energy preserving. The time-dependent Hamilton-Jacobi equation is

$$\frac{\partial S}{\partial t} + H\left(q, \frac{\partial S}{\partial q}\right) = 0$$

with $S(q, q_0, t)$. A canonical transformation $\phi_S : (q_0, p_0) \rightarrow (q, p)$ is generated using

$$p_0 = -\frac{\partial S}{\partial q_0}, \quad p = \frac{\partial S}{\partial q}$$

The initial conditions are chosen so that S generates an identity transformation at $t = 0$

$$S = \frac{1}{2t}(q - q_0)^2$$

The generating function is expanded

$$S = \sum_{i=0}^{\infty} \frac{\Delta t^i}{i!} S_i(p_0, q)$$

and truncated to get an approximate solution S_N . The functions S_i are computed recursively and they satisfy the reversibility condition for canonical Hamiltonian systems with the Hamiltonian $H = \frac{1}{2}p^2 + V(q)$

$$S_i(q, q_0, t) = -S_i(q_0, q, -t)$$

The Ge-Marsden algorithm in [24] is based on a reduction technique which is in fact a symplectic integrator on the symplectic leaves. The resulting scheme preserves the Lie-Poisson structure on the reduced space, i.e. it is symplectic on the symplectic leaves and preserves the angular momentum. Ge-Marsden algorithm is an implicit scheme for general Lie-Poisson systems, but it becomes explicit for the Euler top equations (5). The application of the Ge-Marsden algorithm for the Euler top equations (5) was also given in [24]. Similarly in [23] generating functions are developed for general Poisson maps, which are symplectic on the symplectic leaves. The Ge-Marsden algorithm is then developed using exponential maps in the general Lie algebra setting in [12] and applied to truncated finite dimensional Vasto-Poisson equations. Numerical results show the long term preservation of the energy and therefore the stability of the algorithm. The Ge-Marsden algorithm is composed to obtain higher order Lie-Poisson integrators in [7] and applied again to Vasto-Poisson equations. A modification of the Ge-Marsden algorithm is given in [31] and this is illustrated for the Euler top equation (5).

5.2 Lie-Poisson integrators

The implicit midpoint scheme preserves the constant Poisson structure [46]. It was shown in [5] that the implicit midpoint scheme is an almost Poisson integrator, that it preserves the Lie-Poisson structure up to the second order terms of time step size Δt . The invariance of symplectic difference schemes under symplectic transformations is discussed in [22]. The Hamiltonian function takes different forms in different coordinates, so the symplectic schemes are coordinate dependent, i.e., they are not covariant. This can be shown for the midpoint scheme, which is not invariant under general symplectic coordinate transformations. Let the midpoint scheme for the canonical Hamiltonian system $\dot{u} = J^{-1}H_u$ be

$$\frac{u_{n+1} - u_n}{\Delta t} = J^{-1}H_u \left(\frac{1}{2}(u_n + u_{n+1}) \right) \quad (19)$$

In an another coordinate system v , $u = S(v)$, where S is a symplectic coordinate transformation, the Hamiltonian becomes $H(S(v))$ and the midpoint scheme becomes

$$\frac{v_{n+1} - v_n}{\Delta t} = J^{-1}H_v \left(S \left(\frac{1}{2}(v_n + v_{n+1}) \right) \right) \quad (20)$$

while the original midpoint scheme (19) in the coordinates v is

$$\frac{S(v_{n+1}) - S(v_n)}{\Delta t} = J^{-1}H_v \left(\frac{1}{2}(S(v_n) + S(v_{n+1})) \right) \quad (21)$$

If S is nonlinear then the schemes (20) and (21) are not identical. If S is a linear symplectic transformation $S^T J S = J$, then (20) and (21) are identical. It was shown that some symplectic difference schemes are invariant under certain symplectic coordinate transformations and such schemes are studied for Lie-Poisson systems in [22].

For Lie-Poisson systems in three dimensions, it is more convenient to work with the one form [25]. For the Euler top equation the one form to be preserved becomes [18]

$$J = \sum_{i,j,k} \epsilon_{ijk} J_{ij} dx_k = 2 \sum_{i=1}^3 x_i dx_i \quad (22)$$

It was shown in [18] that (22) is preserved by the symplectic Runge-Kutta methods. Because the energy integral (7) and the total angular momentum (8) of Euler top equation are quadratic, they are preserved exactly by symplectic Runge-Kutta methods of Gauss-Legendry family and by partitioned Runge-Kutta methods of Lobated ILIA-B type. A

detailed comparison of various methods for the rigid body equations can be found in [11].

Explicit Lie-Poisson integrators can be constructed, if the Hamiltonian is separable as for the canonical Hamiltonian systems. The linear structure of flows of Lie-Poisson systems were exploited for the construction of explicit Lie-Poisson integrators [34] and in [49] for the Euler top equation, truncated Vasto-Poisson equations, and Euler equations in fluid dynamics. If the Hamiltonian can be written as $H = \sum_{i=1}^n H_i(x_i)$, then each vector field $X_i = J\nabla H_i$ can be integrated separately by an integrator $\phi_i(\Delta t)$. In the case of the Euler top equation (5) one obtains, with the Hamiltonians $H_i = \frac{x_i^2}{2I_i}$, $i = 1, \dots, 3$, the following splitting:

$$\begin{array}{lll} \dot{x}_1 & = & 0 \\ \dot{x}_2 & = & \frac{x_1 x_3}{I_1} \\ \dot{x}_3 & = & -\frac{x_1 x_2}{I_1} \end{array}, \quad \begin{array}{lll} \dot{x}_1 & = & -\frac{x_2 x_3}{I_2} \\ \dot{x}_2 & = & 0 \\ \dot{x}_3 & = & \frac{x_1 x_2}{I_2} \end{array}, \quad \begin{array}{lll} \dot{x}_1 & = & \frac{x_2 x_3}{I_3} \\ \dot{x}_2 & = & -\frac{x_1 x_3}{I_3} \\ \dot{x}_3 & = & 0 \end{array}$$

A composition of the discrete flows

$$\phi_1(\Delta t) \circ \dots \circ \phi_n(\Delta t)$$

gives a first order explicit integrator for the whole system. A reversible second order composition can also be constructed

$$\phi_1(\Delta t/2) \circ \dots \circ \phi_n(\Delta t) \circ \dots \circ \phi_1(\Delta t/2).$$

The Casimirs, which are the angular momenta of the Euler top equation, are preserved exactly. The Hamiltonian splitting technique was applied to some Lie-Poisson systems, which are obtained as finite dimensional models of some Hamiltonian pde's in plasma physics and fluid dynamics. The truncated Vasto-Poisson equations and the sine-Euler equations [59] as finite dimensional approximations to the two-dimensional Euler equation were integrated in [34] using the Hamiltonian splitting technique and it was shown that all Casimirs are preserved up to the round-off errors. It turns out that explicit Lie-Poisson integrators are by far faster than the Lie-Poisson integrators using generating functions in [12, 24].

Time reversible integrators of arbitrary order were constructed in [29] for some three dimensional bi-Hamiltonian systems like Lotka-Volterra equations, Lorenz equation and for the Toda lattice. Because the Hamiltonians of all these systems are separable for both Poisson brackets, methods based on Hamiltonian splitting can be applied. Symplectic composition of split flows gives an explicit second order time-reversible integrator. Higher order composition techniques [58] are used to increase the order of the methods in [29]. The Hamiltonians are preserved over long time intervals and the periodicity of solutions were retained.

In [20] for nondependence Poisson systems with $2n$ -dimensional symplectic structure $K(x) = J^{-1}(x)$ symplectic difference schemes were constructed using a parameterized nonlinear transformation from the Poisson manifold to the canonical symplectic space. But as stated in [20], in general it is difficult to find parameters which preserve the Poisson structure.

In [60], the integration of Poisson systems with constant Poisson structure is considered and it was concluded that from the class of symplectic Runge-Kutta methods, only the diagonally implicit ones preserve the constant Poisson structure. However Mclachlan pointed out in [35], that because all Runge-Kutta methods are equivalent under linear change of coordinates, the constant structure is also equivalent to a canonical Poisson structure, therefore all symplectic Runge-Kutta methods preserve the constant Poisson structure.

5.3 Semidiscretized Hamiltonian pde's and integrable discretizations

Nonlinear pde's in the Hamiltonian form can be discretized in space, so that the resulting ode inherits the integrals of the pde, this process is known as the integrable discretization. There are some examples of nonlinear pde's like the Landau-Lifschitz equation and the NLS equation, which possess integrable discretized nonlinear lattice equations.

Example 8: Landau Lifschitz equation

The Landau-Lifschitz (LL) equation is a Lie-Poisson Hamiltonian pde [19, 21]

$$\frac{\partial S}{\partial t} = S \times \nabla^2 S + S \times DS \quad (23)$$

and was proposed originally as a model of an anisotropic Heisenberg ferromagnet, where $S = S(x, y, t) \in \mathbb{R}^3$, $\|S\|_2 = 1$ denote the spin length, the matrix $D \in \mathbb{R}^{3 \times 3}$ represents the anisotropy and may be assumed diagonal with $|d_1| \leq |d_2| \leq |d_3|$.

The semi-discretized form of LL on a one-dimensional domain $\Omega = (-L, L)$ gives with $\{x_i \equiv -L + ih, i = 0, \dots, n\}$ the one-dimensional isotropic Heisenberg spin chain

$$\dot{S}_i = \frac{1}{h^2} S_i \times (S_{i-1} + S_{i+1}). \quad (24)$$

The two-dimensional discretized equation over a rectangular domain $\Omega = (-L, L) \times (-L, L)$ with $\{(x_i, y_j) \equiv (-L + ih, -L + jh), i, j = 0, \dots, n\}$, where $h = 2L/n$ and n a positive even integer, has the form

$$\dot{S}_{ij} = S_{i,j} \times M(S_{i,j-1} + S_{i,j+1} + S_{i-1,j} + S_{i+1,j}) \quad (25)$$

where

$$S_{ij} \approx S(ih, jk, t) = \frac{1}{4}(S_{i,j-1} + S_{i,j+1} + S_{i-1,j} + S_{i+1,j})$$

and $M = I/h^2 + D/4$. As boundary conditions periodic or homogenous boundary conditions are taken. The equations (24) and (25) are Lie-Poisson systems and are referred to, for $h = 1$, as lattice Landau Lifschitz (LLL) equations. In two dimensional case, the vector S is defined by using the natural ordering on the grid points:

$$S = [S_{1,1}^T, \dots, S_{1,n}^T, S_{2,1}^T, \dots, S_{2,n}^T \dots S_{n,1}^T, \dots, S_{n,n}^T]^T$$

the equation (25) can be written as a Lie-Poisson system

$$\dot{S} = J(S)\nabla_S H$$

with the Hamiltonian

$$H = - \sum_{i,j} S_{i,j} M(S_{i,j-1} + S_{i,j+1} + S_{i-1,j} + S_{i+1,j}).$$

We use the following notation to describe the form of the structure matrix $J(S)$. For a vector $u \in \mathbb{R}^3$, we associate a 3×3 skew-symmetric matrix $\text{skew}(u)$ such that, for any other vector $v \in \mathbb{R}^3$, $v \times u \equiv \text{skew}(u)v$. Then the structure matrix $J(S)$ consists of blocks of the skew-symmetric matrices $\text{skew}(S_{i,j})$ on the diagonal. The LL equations (24) and (25) have two additional integrals; the individual spin lengths $\|S_{ij}\|_2$ and the total spin length $\sum_i S_i$. This system was integrated for the one dimensional case in [21] by the splitting of the total Hamiltonian $H = - \sum_i S_i \cdot S_{i+1}$ as $H = H_1 + H_2$

$$H_1 = - \sum_i S_i \cdot S_{i+1}, \quad H_2 = - \sum_i S_i \cdot S_{i-1}, \quad \text{for } i \text{ odd}$$

The resulting Lie-Poisson systems

$$\dot{S} = J(S)\nabla H_1, \quad \dot{S} = J(S)\nabla H_2$$

are then integrated with a Lie-Poisson integrator and the corresponding flows are composed in a symmetric form. Another discretization is based on the partitioning of the whole lattice equation. In case of the one dimensional semidiscrete system the spins are ordered as

$$P_i \equiv S_{2i-1}, \quad Q_i \equiv S_{2i}, \quad i = 1, \dots, n/2.$$

We obtain then the following equations

$$\dot{P}_i = P_i \times (Q_{i-1} + Q_i), \quad \dot{Q}_i = Q_i \times (P_i + P_{i+1}), \quad i = 1, \dots, n/2.$$

Defining a vector field splitting $V_H = V_1 + V_2$ by

$$V_1 = \begin{bmatrix} P_1 \times (Q_{n/2} + Q_1) \\ 0 \\ \vdots \\ P_i \times (Q_{i-1} + Q_i) \\ 0 \\ \vdots \\ P_{n/2} \times (Q_{(n-1)/2} + Q_{n/2}) \\ 0 \end{bmatrix}, \quad V_2 = \begin{bmatrix} 0 \\ Q_1 \times (P_1 + P_2) \\ \vdots \\ 0 \\ Q_i \times (P_i + P_{i+1}) \\ \vdots \\ 0 \\ Q_{n/2} \times (P_{n/2} + P_1) \end{bmatrix}$$

one can easily see that each of the vector fields are exactly integrable. This system was integrated in [21] by a semi-explicit staggered scheme which correspond to the second order Lobatto IIIA-B pair [26].

Both methods are time-reversible and preserve the individual lengths of the spin vectors and total spin length. In terms of operation counts the staggered scheme is cheaper than the Lie-Poisson integrator, especially in two and three dimensions.

Example 9: Nonlinear Schrödinger equation

The semi-discretization of the NLS equation (4) by finite differences or by spectral methods and the time integration of the resulting integrable and nonintegrable ode's was the subject of many papers in recent years. The standard finite discretization scheme results in the direct NLS system (DNLS) [2]

$$i\dot{U}_j = -\frac{1}{h^2}(U_{j-1} - 2U_j + U_{j+1}) - 2|U_j|^2 U_j \quad (26)$$

where $h = L/N$ denote the grid spacing. DNLS (26) possesses canonical Hamiltonian structure with the Hamiltonian

$$H = -i \sum_{j=0}^{N-1} \left(\frac{1}{h^2} |U_{j+1} - U_j|^2 - |U_j|^4 \right)$$

and with the only one additional integral of motion (the energy) $I = \sum_{j=0}^{N-1} |U_j|^2$. This system has only two integrals whereas the NLS has infinitely many integrals, therefore the DNLS (26) is not integrable. An integrable discretization of (4) is given by the Ablowitz Ladik discrete NLS equations (IDNLS):

$$i\dot{U}_j = -\frac{1}{h^2}(U_{j-1} - 2U_j + U_{j+1}) - |U_j|^2(U_{j-1} + U_{j+1}) \quad (27)$$

with the Poisson bracket

$$\{q_m, p_n\} = \frac{1}{h}(1 + q_n p_n) \delta_{m,n}, \quad \{q_m, q_n\} = \{p_m, p_n\}$$

the Hamiltonian

$$H = -\frac{i}{h^3} \sum_{j=0}^{N-1} (h^2 p_n (q_{n-1} + q_{n+1}) + 2 \log(1 + h^2 q_n p_n))$$

and an additional first integral

$$I = \sum_{j=0}^{N-1} q_j (p_{j-1} + p_{j+1})$$

where $p_n = U_n$ and $q_n = U_n^*$. The equation (27) has n integrals, i.e. it is completely integrable. The nonintegrable DNLS (26) was integrated in [57] by symplectic Runge-Kutta methods, which preserve the Hamiltonian and the energy integral. The integrable discretization of NLS, the IDNLS equations (27) were transformed in the canonical symplectic form using a Darboux transformation in [57]. The resulting system was then integrated with the symplectic Runge-Kutta methods which preserve the Hamiltonian and the integrals in long-term, whereas the nonsymplectic methods fail.

The integrable discrete NLS equation (27) was integrated in [53] by the construction of a generating function to preserve the Poisson structure. A linear drift in the Hamiltonian error was observed, and it was eliminated by a modification of the scheme in [27].

The following splitting of the Ablowitz-Ladik discrete NLS equations was introduced in [54]:

F^- -flow	F^0 -flow	F^+ -flow
$\dot{q}_n = q_{n-1}(1 - q_n p_n)$	$-2q_n$	$+q_{n+1}(1 - q_n p_n)$
$\dot{p}_n = -p_{n+1}(1 - q_n p_n)$	$+2p_n$	$-p_{n-1}(1 - q_n p_n)$

The flows F^- and F^+ are integrated by the symplectic Euler method and F^0 by the implicit midpoint rule and the whole scheme is obtained by a symmetric decomposition. It was also shown that the Poisson structure for each flow was preserved by the symplectic Euler method [54]. Unfortunately the preservation of the Poisson structure for numerical methods is not independent of the particular equations as in case of the Hamiltonian systems with symplectic structure. A method which is Poisson preserving for one system may not preserve the Poisson structure of another system [54]. The integration above requires, unfortunately, very small step sizes [8], which makes it useless for numerical computations.

Example 10: Volterra lattice equations:

The Volterra lattice equations (16) can also be represented with $u_i =$

y_{2i-1} , $v_i = y_{2i}$ in partitioned form

$$\dot{u}_i = u_i(v_i - v_{i-1}), \quad \dot{v}_i = v_i(u_{i+1} - u_i), \quad i = 1, \dots, m/2 \quad (28)$$

for even m [55]. The equations (28) are also bi-Hamiltonian with the quadratic and cubic Poisson brackets like the original Volterra lattice equations. They were integrated with the partitioned Lobatto IIIA-B methods in [30]. It was shown that the Poisson structure is preserved by the first order symplectic Euler method and by the second order Lobatto IIIA-B methods, whereas any of the Poisson brackets of the Volterra lattice (16) can be preserved by the implicit mid-point method.

Several geometric integrators for the NLS were compared recently in [1], [28], among them the multisymplectic integrators. An alternative formulation of the Hamiltonian pde's involves a local concept of symplecticness in space and in time. Many Hamiltonian pde's are integrated using finite difference and spectral methods by multisymplectic integrators, which show better conservation properties than the symplectic integration of semi-discretized pde's (see for example [50]). An alternative formulation of multisymplecticness and the variational integrators, which are designed to integrate the Hamiltonian pde's are given in [33]. These methods also have good preservation properties. Which geometric integrators are the best for Hamiltonian pde's, is still an open question.

6 Nambu-Hamilton systems and discrete gradient methods

In 1973 Nambu [38] introduced a generalization of the classical Hamiltonian mechanics and an extension of the Poisson bracket. In this formulation, the Poisson bracket is replaced by a ternary or n-ary operation, called Nambu bracket. The underlying idea of this new formulation was that in statistical mechanics the basic result is the Liouville theorem, which follows from but does not require the Hamilton dynamics.

Definition 6 *In the Euclidean space \mathbb{R}^2 with the coordinates x_1 and x_2 the Nambu bracket can be written as*

$$\{F_1, F_2\} = \frac{\partial F_1}{\partial x_1} \frac{\partial F_2}{\partial x_2} - \frac{\partial F_1}{\partial x_2} \frac{\partial F_2}{\partial x_1} = \frac{\partial(F_1, F_2)}{\partial(x_1, x_2)}$$

where this bracket satisfies the Jacobi identity (4). The canonical Nambu bracket is defined for a triple of variables F_1, F_2, F_3 in the phase

space \mathbb{R}^3 with the coordinates x_1, x_2, x_3 by the formula

$$\{F_1, F_2, F_3\} = \frac{\partial(F_1, F_2, F_3)}{\partial(x_1, x_2, x_3)}$$

where the right-hand side stands for the Jacobian.

The first Nambu formulation was given for the Euler top equation with the two Hamiltonians H_1 , the energy integral (7) and H_2 , the total angular momentum (8):

$$\frac{dx}{dt} = \{H_1, H_2, x\} = \nabla H_1 \times \nabla H_2.$$

The Liouville theorem is still valid; the corresponding phase flow preserves the phase space volume. The orbits of a Nambu-Hamilton system in the phase space are determined as the intersection of the surfaces $H_1 = \text{const}$ and $H_2 = \text{const}$. For the Euler top equation, it is given by the intersection of the sphere described by the total angular momentum H_2 , and the total energy H_1 . The trajectories can be found by Jacobi elliptic functions. Nambu introduced also a n -dimensional generalization of the Euler top equation [38]:

$$\begin{aligned} \frac{dx_i}{dt} &= \sum_{jk \dots l} \epsilon_{ijk \dots l} \frac{\partial H_1}{\partial x_j} \frac{\partial H_k}{\partial x_k} \dots \frac{\partial H_{n-1}}{\partial x_k}, \\ \frac{dx}{dt} &= \frac{\partial(x, H_1, \dots, H_{n-1})}{\partial(x_1, \dots, x_n)} \end{aligned}$$

where $\epsilon_{ijk \dots l}$ denotes the Levi-Civita tensor. In 1994 Takhtajan [56] made a geometric formulation of Nambu-Poisson bracket, which satisfies the skew symmetry, Leibniz rule and the fundamental identity, which is a generalization of the Jacobi identity. According to [56], the dynamics on the Nambu-Poisson manifold is determined by $n - 1$ Hamiltonians H_1, \dots, H_{n-1} and is described by the generalized Nambu-Poisson equation:

$$\frac{dx}{dt} = \{H_1, \dots, H_{n-1}, x\}$$

The fundamental identity is given the $n = 3$ as

$$\begin{aligned} \{\{G, H, F_1\}, F_2, F_3\} &+ \{F_1, \{G, H, F_2\}, F_3\} + \{F_1, F_2, \{G, H, F_1\}, F_3\} \\ &= \{G, H, \{F_1, F_2, F_3\}\}. \end{aligned}$$

A function F is called an integral of motion for the Nambu-Hamilton system if its Nambu bracket with the Hamiltonians H_1, \dots, H_{n-1} vanishes. A Nambu bracket of n integrals of motion is again an integral of motion, this shows that many integrable systems possess Nambu structure.

Example 11: Lagrange system:

The so called Lagrange system [56] which occurs in $SU(2)$ monopoles on \mathbb{R}^3

$$\dot{x}_1 = x_2 x_3, \quad \dot{x}_2 = x_3 x_1, \quad \dot{x}_3 = x_1 x_2$$

can be written in the Nambu form

$$\dot{x}_i = \{x, H_1, H_2\}, \quad H_1 = \frac{1}{2}(x_1^2 - x_2^2), \quad H_2 = \frac{1}{2}(x_1^2 - x_3^2).$$

It turned out that many physical systems can be written in Nambu form; like the Halpen system [56], some vortex equations in fluid dynamics [6], some two dimensional incompressible flow equations [43], $SU(n)$ isotropic harmonic oscillators and the $SO(4)$ Kepler problem [14]. The three dimensional Lotka-Volterra equations (12) also can be written in Nambu form

$$\dot{x} = M(x) \nabla H_1 \times \nabla H_2$$

where $M(x) = x_1 x_2 x_3$ with the Hamiltonians H_1 and H_2 in (13).

Poisson systems can also be considered as a special case of a discrete gradient system [36]

$$\dot{x} = S(x) \nabla I(x) \quad (29)$$

where $S(x)$ is skew-symmetric and $I(x)$ is a first integral. The integral preserving methods based on the construction of discrete gradients in [37, 47] are similar to those conserving schemes for Hamiltonian systems. The discrete gradient method consists of the replacement of the continuous gradient $\nabla I(x)$ by the discrete gradient $\bar{\nabla} I(x)(x, \hat{x})$ which satisfies

$$\begin{aligned} \bar{\nabla} I(x)(x, \hat{x})(\hat{x} - x) &= V(\hat{x}) - I(x), \\ \bar{\nabla} I(x)(x, \hat{x}) &= \nabla I(x) + O(\hat{x} - x). \end{aligned}$$

The resulting discrete gradient system can then be constructed as

$$\frac{\hat{x} - x}{\Delta t} = \tilde{S} \bar{\nabla} I(x)(x, \hat{x})$$

where \tilde{S} is any consistent skew-symmetric matrix such that $\tilde{S}(x, \hat{x}) = S\left(\frac{x+\hat{x}}{2}\right)$. It can be easily seen from the skew-symmetry of \tilde{S} , that the first integrals are preserved, i.e. $I(x) = I(\hat{x})$. Discrete gradients are not unique; several examples of them are given in [37, 47].

Systems with multiple integrals $I_1(x), \dots, I_{n-1}(x)$ like the Nambu systems (6) can be written in the multi-gradient form

$$\dot{x} = S(x) \nabla I_1(x) \cdots \nabla I_{n-1}(x)$$

where $S(x)$ is an n skew-symmetric tensor. Discrete gradient systems which preserve the multiple gradients can be constructed similarly [36].

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